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Exact Coulomb corrections in beta decay and inner bremsstrahlung

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Abstract : In order to explain the existing discrepancy between the experimental and theoretically computed Inner Bremsstrahlung (IB) spectra, it is intended to incorporate exact Coulomb factor in the IB expressions and examine whether the nuclear charge has any influence on the IB spectrum Due to the complexity of the Fermi Coulomb correction factor $F(Z,W)$, several approximations and numerical tables for selected momentum (p) values are available in literature In this paper, a simple and highly accurate quadrature method is developed for the evaluation of $F(Z,W)$ The method has been validated against well known analytic expressions for some specific values It is seen that with six nodes in the gaussian quadrature, the computed results agree with exact value to better than six significant digits A comparative analysis of the earlier published approximations and tabulated values with present calculation deemed to be exact, is given in the paper When incorporated into the theoretical IB spectral distribution, the improvement has been only marginal and the discrepancy between the theory and the reported experimental data still remains

Keywords : Fermi function, exact Coulomb correction, inner bremsstrahlung (IB)

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1. Introduction

The influence on the beta spectrum by the Coulomb field of the nucleus on the outgoing beta particle in Beta decay is given by the Fermi function [1] as

$$F(Z,W) = \frac{2(1+S)(2\rho p)^{(2S-2)} e^{\pi\eta} |\Gamma(S+i\eta)|^2}{[\Gamma(2S+1)]^2} \tag{1}$$

where $S = (1 - \alpha^2 Z^2)^{1/2}$,

Z = atomic number of the daughter nucleus,

α = fine structure constant = 1/137.04,

$\rho = R/(\hbar/mc)$,

R = r.m.s. radius of the nucleus (assuming uniform charge distribution

$R = 1.45A^{(1/3)}$, A being the Mass number),

W = Energy of the beta particle in relativistic units,

P = Momentum of the beta particle in relativistic units, $p = (W^2 - 1)^{1/2}$

$\eta = \alpha ZW/p$ and $\Gamma(2S + 1)$ and $\Gamma(S + i\eta)$ are Gamma functions.

Due to the presence of the complex hypergeometric function, exact evaluation of $F(Z,W)$ poses severe difficulties. In view of this, several approximations have been suggested for the Fermi function. Mott and Massey [2] gave a non-relativistic approximation in the form

$$F(Z,W) = 2\pi\eta \,/\, [1 - e^{-2\pi\eta}]. \qquad (2)$$

For low Z, the expression reduces to

$$F(Z,W) = 1 + \pi\alpha ZW / p. \qquad (3)$$

Using the asymptotic expansion of the Gamma (Γ) function, Hall [3] gave the expression

$$F(Z,W) = \frac{4\pi(1+S)(2p\rho)^{(2S-2)}\left(S^2+\eta^2\right)^{(S-1/2)} e^{(2\phi\eta - 2S)}\left[1+\left\{S/6(S^2+\eta^2\right)\right.}{\left[\Gamma(2S+1)\right]^2}$$

where $\phi = \tan^{-1}(S/\eta)$.

Nilsson [4] gave an empirical relation

$$F(Z,W) = aW/p + C/(1 + d/p^2),$$

where $a = 2\pi\alpha Z$, $C = b - a$, $b = a/(1 - e^{-a})$, $d = (b - 1)/2$.

Bethe and Bacher's [5] approximation is

$$F(Z,W) = \frac{4(1+S)\rho^{2S-2}\pi\eta\left[W^2(1+4\alpha^2Z^2)-1\right]^{(S-1)}}{(1-e^{-2\pi\eta})\{\Gamma(2S+1)\}^2}$$

Numerical evaluation of Fermi function has been done for selected values of p over a wide range and tabulated by several workers [6–17]. All these calculations have assumed uniform charge distribution in the nucleus. For values of p other than those given in the tables, a nonlinear interpolation has to be made. Rose [6] tabulated the modified Fermi function $G = F(Z,W)p/W$ for each Z over a wide range of momenta. Using these tabulated values and linear regression method, Venkataramaiah *et al* [18] obtained a simple formula for the Fermi function as

$$F(Z,W) = \left[A + \{B/(W-1)\}\right]^{1/2},$$

where A and B are the constants for a given beta emitter. This is said to reproduce the tabulated values of Fermi function to an accuracy of 1% for $p \geq 25$ KeV/c.

The inclusion of the Coulomb correction in beta decay and the IB spectral distribution accompanying beta decay, require the integration of a complex expression containing Fermi function as a multiplier. Evaluation of such an integral demands the representation of the Fermi function in a manageable form. Therefore, an attempt has been made to arrive at an easily calculable form of Fermi function without approximations for the desired energy/momenta of the electron in beta decay.

2. Computation of the Fermi function

In the calculation of the Fermi function [eq. (1)], the problem is in the computation of the factor

$$f(S,\eta) = e^{\pi\eta}\,|\Gamma(S+i\eta)|^2.$$

As W approaches the rest mass of the electron, $\eta \to \infty$. Hence, $e^{\pi\eta} \to \infty$ but $|\Gamma(S+i\eta)|^2 \to 0$. Computing them independently and then taking the product, could lead to numerical errors and hence there is the need to treat them together.

To compute $f(S,\eta)$, we proceed as follows.

We have (from [19])

$$\frac{1}{\beta(m,n)} = \frac{(1/\pi)2^{m+n-2}(m+n-1)\int_0^{\pi}\cos[t(m-n)]\sin^{m+n-2}t\,dt}{\cos\{(m-n)\pi/2\}},$$

also

$$\frac{1}{\beta(m,n)} = \frac{(1/\pi)2^{m+n-2}(m+n-1)\int_0^{\pi}\sin[t(m-n)]\sin^{m+n-2}t\,dt}{\sin\{(m-n)\pi/2\}},$$

$$\Gamma(m)\Gamma(n) = \Gamma(m+n)\beta(m,n), \text{ and } z\,\Gamma(z) = \Gamma(z+1),$$

where m, n and z are real or complex numbers and $\beta(m,n)$ is the Beta function. With $z = S + i\eta$, $m = S + i\eta + 1$ and $n = S - i\eta + 1$ in the above expressions and a little algebra, we get

$$|\Gamma(S+i\eta)|^2 = (2S+1)\,\Gamma(2S+1)\,\beta(S+i\eta+1, S-i\eta+1)/(S^2+\eta^2) \quad (8)$$

and

$$\frac{e^{-\pi\eta}}{\beta(S+1+i\eta, S+1-i\eta)} = \frac{2^{2S}(2S+1)}{\pi}\int_0^{\pi} e^{-2\eta t}\,\sin^{2S} t\,dt. \quad (9)$$

The integral in eq. (9) is quite amenable for numerical integration by Gaussian quadrature except when η is very large. For $\eta \gg 1$ the integrand tends to get concentrated near $t = 0$ and any number of quadrature points in the numerical integration fail to properly span the integrand. Hence for large values of η, setting $r = 2\eta t$, the eq. (9) takes the form

$$\frac{e^{-\pi\eta}}{\beta(S+1+i\eta, S+1-i\eta)} = \frac{2^{2S}(2S+1)}{2\pi\eta}\,I, \quad (10)$$

where,

$$I = \left\{\sum_{n=0}^{N-1}\int_{n\pi}^{(n+1)\pi} F(r)dr\right\} + \left\{\int_{N\pi}^{2\eta\pi} F(r)dr\right\},$$

where $F(r) = e^{-r}\sin^{2S}(r/2\eta)$, and N is the integer part of 2η.

Writing $r = U + n\pi$, we get

$$I = \left\{ \sum_{n=0}^{N-1} {}_0\!\int^{\pi} F(U)dU \right\} + \left\{ {}_0\!\int^{(2\eta - N)\pi} F(U)dU \right\}, \tag{11}$$

where $F(U) = e^{-(U+n\pi)} \sin^{2S}[(U+n\pi)/2\eta]$.

In this form, the integrals in the expression for I have the desired future; they span the right region for all η. With increasing η, the number of terms in the summation increases. However since the integrals are multiplied by $e^{-n\pi}$ or $e^{-N\pi}$, the summation has a very fast convergence, with $n = 2$ being adequate for an error of less than 0.1%. Using the expression (10) for the β function in expression (8) and with the use of eq. (11) for I, we obtain using expressions 11, 10 and 8 in eq. (1), we obtain

$$e^{\pi\eta} |\Gamma(S+i\eta)|^2 = \frac{2^{(1-2S)} \pi\eta\Gamma(2S+1)}{(S^2+\eta^2)I} \tag{12}$$

and

$$F(Z,W) = \frac{2^{2-2S} \pi\eta (1+S)(2p\rho)^{2S-2}}{\Gamma(2S+1)(S^2+\eta^2)I} \tag{13}$$

To validate expression (12), it has been computed for $S = 0$, 0.5 and 1.0 for which closed form expressions exist (Gradshteyn and Ryzhik [19]). The comparison is given in Table 1

Table 1. Accuracy in the present method of computation when used to compute known closed complex gamma functions

Function $\rightarrow \eta$	$e^{\pi\eta}\|\Gamma(0+i\eta)\|^2$	$e^{\pi\eta}\|\Gamma(0.5+i\eta)\|^2$	$e^{\pi\eta}\|\Gamma(1+i\eta)\|^2$
0 1	0 (0)*	5.8E–5 (3 5E–5)	2E 4 (08)
0 5	0 (3 8E-4)	3.7E–5 (1 06E–2)	1.67E-4 (22)
1 0	0 (7 6E–4)	7 6E–6 (4 5E–4)	0 (5 2E -4)
5 0	9 5E–6 (3 8E–4)	0 (2 5E–3)	1 8E–5 (6 5E 3)
10 0	9.5E–6 (3 8E–4)	0 (2 5E–3)	0 (6 5E 3)
50 0	1 2E–5 (3 8E–4)	7 6E–6 (2.5E–3)	0 (6 5E–3)
100 0	1 2E-5 (3.8E–4)	7 6E–6 (2 5E–3)	0 (6 5E 3)
200.0	1.2E–5 (3 8E–4)	0 (2 5E–3)	0 (6 5E–3)

*Percentage error in numerical computation by Gaussian method with six Nodes (the numbers in the parenthesis represent the percentage error with four Nodes)

As can be seen from the table, even with only four quadrature points, eq. (12) agrees with the exact values to better than 0.1% and with six quadrature points the agreement to better than six significant digits. In view of this high accuracy, the present results are taken to be exact in subsequent discussion.

The variation of $F(Z,W)$ with Beta kinetic energy, calculated using different approximations is shown in Figures (1–3). The Z-values chosen are in the range in which most of the experimental IB results exist. The modified Fermi function $G(Z,p) = F(Z,W)p/W$

for different approximations are compared with the present results for various values of p and Z in Table 2. The empirical formula [18], agrees fairly well with the computed exact

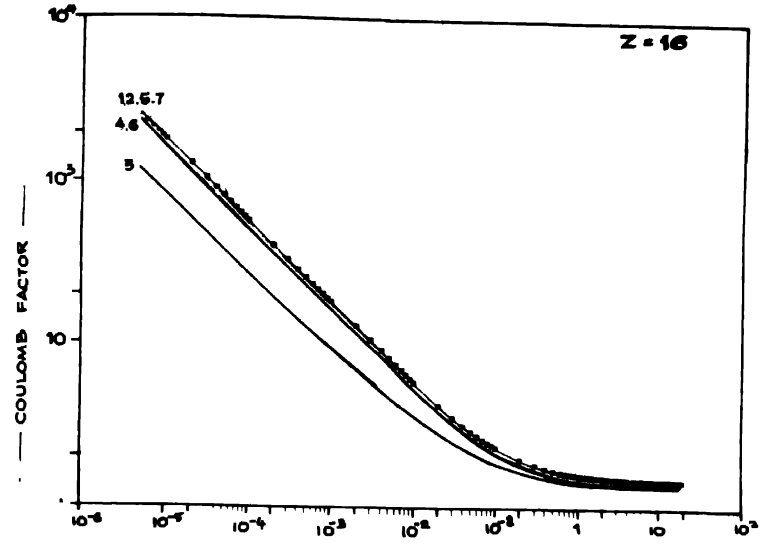

Figure 1. Coulomb correction factor $F(Z,W)$ for $Z = 16$ 1 exact, 2 Venkataramaiah *et al* [18], 3 Mott and Massey approximation for low Z [2], 4. Mott and Massey non relativistic approximation [2], 5 Hall approximation for low momentum [3], 6 Nilsson empirical formula [4], 7 Bethe and Bacher's non relativistic approximation [5]

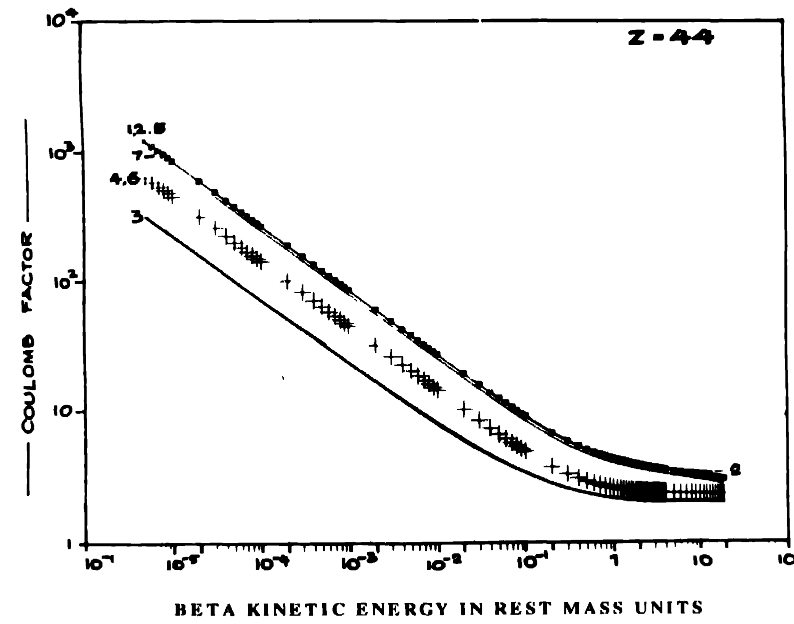

Figure 2. Coulomb correction factor $F(Z,W)$ for $Z = 44$. 1 exact, 2 Venkataramaiah *et al* [18], 3. Mott and Massey approximation for low Z [2], 4. Mott and Massey non relativistic approximation [2], 5. Hall approximation for low momentum [3], 6 Nilsson empirical formula [4], 7. Bethe and Bacher's non relativistic approximation [5]

Fermi function within an accuracy of better than 2% for low and medium Z over a wide range of the energies (upto about 2 MeV for $Z = 16$ and $Z = 44$). Fairly good agreement exists for high Z too (for example, upto about an MeV for $Z = 75$).

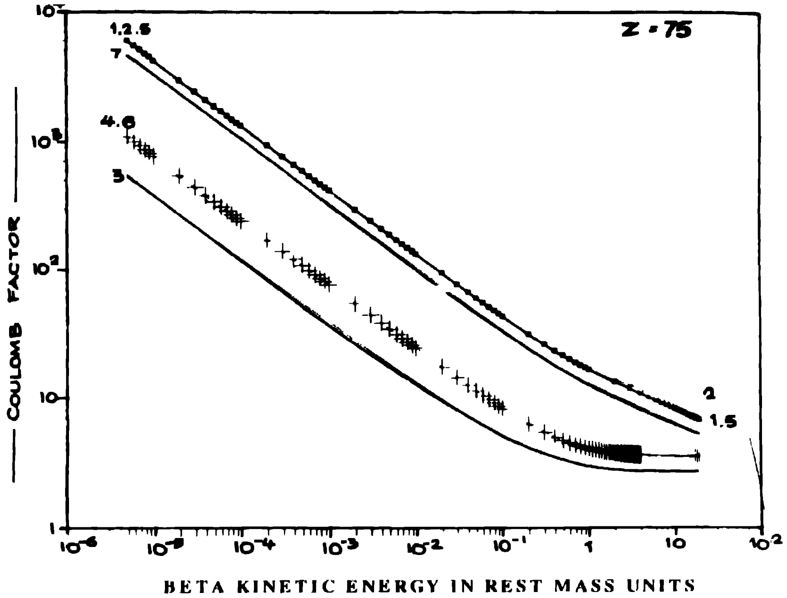

Figure 3. Coulomb correction factor $F(Z,W)$ for $Z = 75$ 1. exact, 2. Venkataramaiah *et al* [18], 3 Mott and Massey approximation for low Z [2], 4 Mott and Massey non relativistic approximation [2], 5 Hall approximation for low momentum [3], 6. Nilsson empirical formula [4], 7 Bethe and Bacher's non relativistic approximation [5]

Table 2. Comparison of exact Coulomb factor with other approximations

	$Z = 16$ ($A = 35$)				$Z = 44$ ($A = 102$)				$Z = 75$ ($A = 187$)			
P	Exact	Hall	Rose	Venkataramaiah *et al*	Exact	Hall	Rose	Venkataramaiah *et al*	Exact	Hall	Rose	Venkataramaiah *et al*
1	0.811	0.808	0.813	0.791	3.816	3.815	3.835	3.795	18.72	18.71	18.93	19.06
5	0.994	0.986	0.995	0.988	3.750	3.726	3.764	3.800	17.88	17.82	18.05	18.14
7	1.106	1.097	1.107	1.100	3.744	3.717	3.758	3.794	17.24	17.15	17.40	17.45
1.0	1.230	1.221	1.231	1.233	3.750	3.720	3.763	3.776	16.29	16.18	16.45	16.42
2.0	1.406	1.395	1.407	1.428	3.698	3.667	3.710	3.683	13.88	13.76	14.01	14.04
3.0	1.454	1.442	1.455	1.483	3.606	3.576	3.618	3.607	12.37	12.26	12.48	12.84
4.0	1.470	1.458	1.471	1.504	3.523	3.494	3.535	3.556	11.33	11.23	11.44	12.17
6.0	1.478	1.466	1.479	1.517	3.393	3.365	3.405	3.493	9.974	9.886	10.07	11.45
7.0	1.478	1.467	1.479	1.519	3.342	3.314	3.353	3.474	9.495	9.411	9.587	11.24
9.0	1.477	1.466	1.478	1.521	3.258	3.232	3.270	3.446	8.757	8.680	8.843	10.96
13.0	1.473	1.461	1.474	1.522	3.137	3.111	3.148	3.414	7.774	7.706	7.851	10.65
15.0	1.471	1.459	1.472	1.522	3.091	3.065	3.102	3.404	7.421	7.356	7.494	10.55

The Hall approximation compares very well with the exact $F(Z,W)$ for all Z over a wide energy range. A discrepancy of about one percent occurs at around 10 MeV of electron kinetic energy. Bethe and Bacher's non-relativistic approximation bears a constant ratio with exact F for all energies for a given Z (a ratio of 0.99 for $Z = 16$, 0.93 for $Z = 44$ and 0.785 for $Z = 75$). The Mott and Massey equation and its low Z approximation appear to run parallel to the exact F upto a certain extent, and tends to reach a constant value at about 150 KeV.

All the Coulomb correction expressions discussed above, when used in the IB probability expressions normalised with respect to the total beta intensity, yield very nearly identical results. Wherever absolute quantity of F is required, the choice should be between the empirical equation of Venkataramaiah *et al* [18] and the equation of Hall as the discrepancy between the exact value and the approximations suggested by others is found to be more as illustrated in the Figures (1–3). The former is suggested due to its simplicity as well as accuracy for low and medium Z for all energies and for relatively high Z upto a kinetic energy of 1.5 MeV. The Hall equation requires the calculation of a Γ-function and is suggested particularly, when the kinetic energy in question is more than 1.5 MeV for a given high Z isotope.

3. Computation of IB spectral distribution

Knipp and Uhlenbeck [20] and Bloch [21] calculated the IB spectrum for allowed transitions (KUBA) assuming no influence from the nuclear charge. Later, Lewis and Ford [22] modified the KUB theory including a first order Coulomb correction due to Mott and Massey (low Z approximation) (LFA). They also calculated the IB spectrum for the case of Unique First Forbidden transitions with similar Coulomb correction (LFFF). Ford and Martin [23] incorporated the Detour transitions in addition to direct transitions into the FFFF (FMFF). Chang and Falkoff [24] calculated the IB intensities in the second forbidden transitions without Coulomb correction (CFSF). To calculate the No. of IB photons per beta disintegration per unit energy range $S(k)$, the absolute IB intensities were normalised to the total beta intensities calculated for respective degree of forbidden-ness

The IB emission probability distribution expressions given by KUBA, LFA, LFFF, FMFF and CFSF are used in the computation of the IB intensities incorporating the exact Coulomb correction into both IB and beta intensity integrals. $S(k)$ is given by

$$S(k) = \frac{\int_1^{W_0-k} F_1(\mathrm{IB}) F(Z,W) dW}{\int_1^{W_0} F_2(\mathrm{beta}) F(Z,W) dW}$$

where $F_1(\mathrm{IB})$ represents in general, the probability of the emission of a photon of energy k associated with the beta particle carrying a kinetic energy greater than k per unit beta kinetic energy range, as described by any one among KUBA, LFFF, FMFF or CFSF whichever is appropriate to the transition of a given type. F_2(beta) is the probability of the beta emission per unit beta kinetic energy interval appropriate to the degree of forbidden-ness. W_0 is the end point energy in relativistic units and W is the energy of the beta particle far away from the nucleus.

It can be seen from the Figure 4 that the variation of calculated intensity (for a particular type of transition) varies only marginally between $Z = 0$ ($F(Z,W) = 1$) approximation and the incorporation of exact $F(Z,W)$. The first order Coulomb corrected spectrum ($F(Z,W) = 1 + \pi\eta$) lies in between these two. The experimental spectrum is also shown.

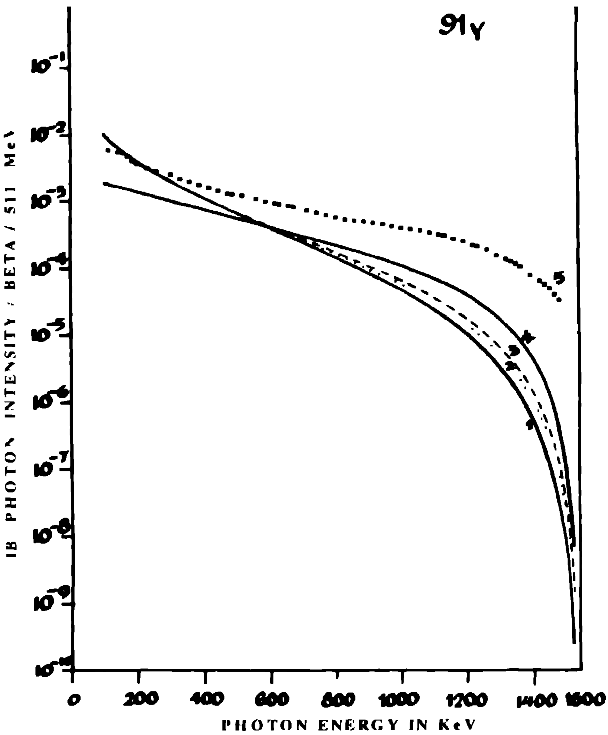

Figure 4. IB spectrum of ^{91}Y 1 LFFF with $Z = 0$ approximation 2 LFFF with $F(Z,W) = 1 + \pi\eta$ 3 LFFF with exact $F(Z,W)$, 4 CTSI with exact $F(Z,W)$, 5. Experimental spectrum [31]

Several experimentalists reported discrepancy between the theory and the experiment, particularly towards the high energy end of the spectrum {^{32}P and ^{35}S [22], ^{36}Cl [25], ^{185}W and ^{90}Y [26], ^{111}Ag [27], ^{63}Ni [28]), ^{86}Rb [29], ^{147}Pm [30], ^{91}Y and ^{89}Sr [31] ^{141}Ce [32] and ^{99}Tc [33], *etc.*}. The computed values using the appropriate expressions as mentioned above, are always lower than the measured ones at the higher energy region. The low intensity of IB require long counting hours to get statistically significant results. The raw count rates in the high energy region are closer to the background count rates. Hence the difference between a mean raw source count rate and the corresponding mean background count rate, which is statistically significant at 68% confidence level may turnout to be insignificant at 95% level. It is the normal practice to use 68% confidence level in nuclear counting which is good enough for high source count rates. Hence there exists a possibility of decision making error with the choice of significance level

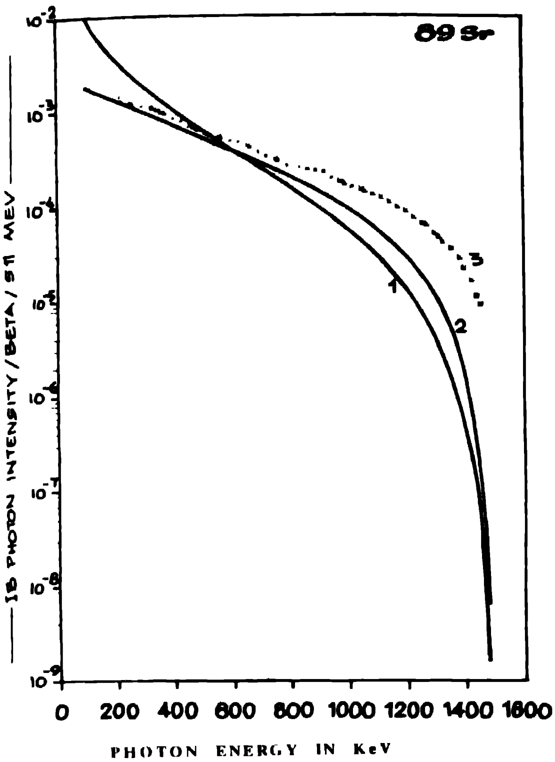

Figure 5. IB spectrum of ^{89}Sr : 1. LFFF with exact F(Z,W), 2. CFSF with exact $F(Z,W)$, 3 Experimental spectrum [31].

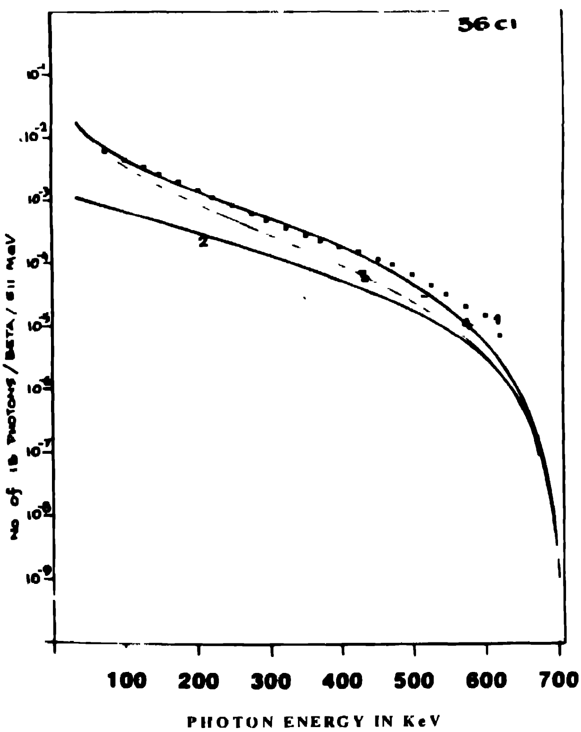

Figure 6. IB spectrum of ^{36}Cl
1 Experimental spectrum [25],
2. CFSF with exact $F(Z,W)$,
3 LFFF with exact $F(Z,W)$,
4. FMFF with exact $F(Z,W)$

During the course of this study, we found some interesting points. The experimental IB spectrum of ^{91}Y and ^{89}Sr whose beta transitions are classified as 1st forbidden, run parallel to the second forbidden theoretical results of Chang and Falkoff (Figures 4 and 5). Further the experimental IB spectrum of ^{36}Cl whose nuclear transformation is classified as second forbidden, is closer to Ford and Martin theory for 1st forbidden transition (Figure 6). These observations possibly suggest that the IB spectrum could be of some help in classifying the degree of forbidden-ness in beta decay.

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